

11 December 2002**ROBUST SUMMARY FOR 1,5-CYCLOOCTADIENE**Summary

1,5-Cyclooctadiene is a colorless liquid with an aromatic odor and molecular weight of 108.20. It has a melting point of  $-70$  to  $-69^{\circ}\text{C}$ , a boiling point of  $150.8^{\circ}\text{C}$  at 757 mm Hg, specific gravity of 0.8818 at  $25/4^{\circ}\text{C}$ , and vapor pressure of 6.8 mm Hg at  $25^{\circ}\text{C}$ . 1,5-Cyclooctadiene is a flammable liquid with an autoignition temperature of  $223^{\circ}\text{C}$  and a flash point of  $35^{\circ}\text{C}$ . The octanol/water partitioning coefficient (log Kow) was determined to be 3.16. The bioconcentration factor (BCF) was estimated as 54.1, based on the empirical log Kow of 3.16; therefore, the potential for this compound to bioaccumulate is in the low to moderate range. Based on the measured log Kow, the estimated water solubility is 64.11 mg/L.

A Henry's Law constant of  $1.101 \times 10^{-2}$  atm-m<sup>3</sup>/mole was estimated based on an estimated vapor pressure of 4.96 mm Hg and an estimated water solubility of 64.1 mg/L. The test substance is expected to have a half-life in air of 0.568 hours, with equal emissions to air, water, and soil. The estimated half-life in air as a result of reaction with OH radicals is estimated as 3.28 hours; with ozone the half-life is estimated as 41.256 minutes. Fugacity model predictions indicate that 1,5-cyclooctadiene will partition mainly to water and soil when emitted equally to air, water, and soil. Less than 2% will partition to air and sediments. Primary biodegradation is estimated to occur in days to weeks. Ultimate biodegradation is estimated to occur in weeks.

1,5-Cyclooctadiene was moderately toxic to aquatic fish and highly toxic to invertebrates with a 48- and 96-hour LC<sub>50</sub> in rainbow trout of 30-38 mg/L, and a 24-hour LC<sub>50</sub> in *Daphnia* of 0.9 mg/L. Based on ECOSAR predictions, 1,5-cyclooctadiene would have a 96-hour EC<sub>50</sub> in green algae of 5.0 mg/L. ECOSAR predictions are generally substantiated by comparing the values obtained in the model to those obtained from actual testing of an analogous compound. Since no measured test data for an analogous chemical were available, an algae study is recommended to determine the actual algal toxicity potential of this test substance.

1,5-Cyclooctadiene had an oral LD<sub>50</sub> in rats of 2.7 mL/kg. It was slightly toxic to rats via the inhalation route with a 4-hour ALC (approximate lethal concentration) of 2700 ppm and moderately toxic via the dermal route with a dermal LD<sub>50</sub> of  $> 3520$  mg/kg. 1,5-Cyclooctadiene was a skin and eye irritant and a potent skin sensitizer. In a 2-week inhalation neurotoxicity study in rats at doses of 0, 50, 150, and 500 ppm, the NOEL (no-observed-effect level) was 150 ppm, based on decreased alerting response in rats during exposure and effects in the nose, kidneys, and urine of rats exposed to 500 ppm. No test substance-related findings in neuropathologic evaluation were observed at any level tested. No information regarding developmental or reproductive toxicity was available; therefore, a combined repeated dose toxicity study with the reproduction/developmental toxicity screening test (OECD Guideline 422) is recommended.

1,5-Cyclooctadiene was negative for mutagenicity in *Salmonella typhimurium* and *E. coli*, negative for clastogenicity in human lymphocytes, and negative in an *in vivo* rat micronucleus assay.

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**Exposure Assessment for 1,5-Cyclooctadiene**

1,5-Cyclooctadiene is manufactured at one DuPont facility. 1,5-Cyclooctadiene is a co-product produced in the manufacture of cyclododecatriene. 1,5-Cyclooctadiene is used as a chemical intermediate for the production of flame retardants, aroma chemicals, catalysts, and rubber goods.

The potential for exposure is the greatest during the loading and unloading of 1,5-cyclooctadiene since closed processes are used on the site. The site can have approximately 1100 personnel working (construction, contractor, and plant employees). The areas where the substance is manufactured will have 16 total operators during normal operations and 40 people during a shutdown or major construction activity.

The site has effective safety, health, and environmental practices and procedures in addition to engineering controls, environmental controls, and personal protective equipment to control exposure. Adequate safety equipment, such as safety showers, eyewash fountains, and washing facilities, are available in the event of an occupational exposure. Individuals handling 1,5-cyclooctadiene should wear safety glasses and impervious clothing, such as gloves, apron, boots, or whole bodysuit made of nitrile rubber or Viton. When the possibility exists for eye and face contact due to splashing or spraying of material, chemical splash goggles and face shield should be worn. DuPont practices responsible care and assesses the ability of potential customers to safely handle 1,5-cyclooctadiene prior to commencing a commercial relationship. The Product Stewardship System works with customers to understand their applications and any issues associated with PPE (personal protective equipment), safety equipment (safety showers, eyewash stations, ventilation needs, etc.), storage concerns, disposal requirements, and MSDS questions.

Air monitoring has been conducted on 1,5-cyclooctadiene using the site Industrial Hygiene Procedure (OSHA 07). LOGAN (lognormal analysis) is a computerized statistical method for characterizing occupational exposures to chemicals, noise, and other environmental hazards. LOGAN uses sequential collection of data and makes decisions on the minimum amount of data. It helps make cost-effective, accurate decisions that ensure a healthy workplace. LOGAN uses inferential statistics to estimate the true workplace conditions, in the same way that public polling estimates opinions by sampling a representative percentage of the public. LOGAN is designed to limit the risk of employee occupational overexposure to less than 5%.

The DuPont Acceptable Exposure Limit for 1,5-cyclooctadiene is 10 ppm, 8- and 12-hour TWA. No other limits have been established. None of the samples taken suggest the probability of exposure in excess of the current recommended AEL of 10 ppm, 8- and 12-hour TWA.

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**EXPOSURE DATA**

**Area: Operators and Maintenance**

	People	No. of Results	Avg. of TWA (ppm)	Min. of Results (ppm)	Max. of TWA (ppm)
Production	16 (since 1990)	403	0.07	<0.01	2.47
Maintenance	30 (since 1990)	153	0.13	<0.01	0.13

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**TEST PLAN FOR 1,5-CYCLOOCTADIENE**

<b>1,5-Cyclooctadiene</b> <b>CAS No. 111-78-4</b>	<b>Data Available</b>	<b>Data Acceptable</b>	<b>Testing Required</b>
	<b>Y/N</b>	<b>Y/N</b>	<b>Y/N</b>
<b>PHYSICAL/CHEMICAL CHARACTERISTICS</b>			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
<b>ENVIRONMENTAL FATE</b>			
Photodegradation	Y	Y	N
Stability in Water	Y	Y	N
Transport (Fugacity)	Y	Y	N
Biodegradation	Y	Y	N
<b>ECOTOXICITY</b>			
Acute Toxicity to Fish	Y	Y	N
Acute Toxicity to Invertebrates	Y	Y	N
Acute Toxicity to Aquatic Plants	N	N	Y
<b>MAMMALIAN TOXICITY</b>			
Acute Toxicity	Y	Y	N
Repeated Dose Toxicity	Y	N	Y
Developmental Toxicity	N	N	Y
Reproductive Toxicity	N	N	Y
Genetic Toxicity Bacterial Gene Mutations	Y	Y	N
Genetic Toxicity <i>in vitro</i> Chromosomal Aberrations	Y	Y	N
Genetic Toxicity <i>in vivo</i> Micronucleus	Y	Y	N